(A) using atomic coordinates obtained from crystallographical analysis of a TACE polypeptide to design an associating compound that forms a bond with the catalytic domain of said TACE polypeptide; and

(B) determining whether said compound associates with said TACE polypeptide,

wherein said atomic coordinates comprise the coordinates of Table 1, or a substantial part thereof, and said TNF-α-converting enzyme polypeptide comprises the TNF-α-converting enzyme catalytic domain,

further wherein said associating compound is a TACE inhibitor.

65. A method of identifying a compound that associates with tumor necrosis factor-α-converting enzyme (TACE), comprising:

(A) using atomic coordinates obtained from crystallographical analysis of a TACE polypeptide to design an associating compound that forms a bond with the catalytic domain of said TACE polypeptide; and

(B) determining whether said compound associates with said TACE polypeptide,

wherein said atomic coordinates comprise the coordinates of Table 1, or a substantial part thereof, and said TNF-α-converting enzyme polypeptide comprises the TNF-α-converting enzyme catalytic domain,

further wherein said associating compound is designed to introduce a non-polar group which occupies the S1' pocket of TNF-α-converting enzyme.

Please amend the following claims:

41. (Amended) The method according to claim **[40]** **63**, wherein said associating compound is an inhibitor, mediator, or other compound that regulates TNF-α-converting enzyme activity.

43. (Amended) The method according to claim **[40]** **63**, wherein the coordinates **[are]** **comprise** the coordinates of Table 1, or a substantial part thereof.

44. (Amended) The method according to claim **[40]** **63**, wherein said TNF-α-converting enzyme polypeptide **[crystal]** comprises the TNF-α-converting enzyme catalytic domain.

45. (Amended) The method according to claim **[40]** **63**, wherein said TNF-α-converting enzyme polypeptide is the expression product of a polynucleotide encoding the pro and catalytic domains of TNF-α-converting enzyme.

46. (Amended) The method according to claim **[40]** **63**, wherein said TNF-α-converting enzyme polypeptide is the expression product of a polynucleotide encoding the amino acid residues 1-477 of TNF-α-converting enzyme.

48. (Amended) The method according to claim **[40]** **63**, wherein said TNF-α-converting enzyme polypeptide **[crystal]** is co-crystallized with a binding partner.

51. (Amended) The method according to claim **[40]** **63**, wherein said TNF-α-converting enzyme polypeptide **[crystal]** has a crystal structure diffracting to 2.0 Å.

52. (Amended) The method according to claim **[40]** **63**, wherein **the crystal of** said TNF-α-converting enzyme polypeptide **[crystal]** is monoclinic.

53. (Amended) The method according to claim **[40]** **63**, wherein **the crystal of** said TNF-α-converting enzyme polypeptide **[crystal]** has a unit cell comprising four crystallographically independent TNF-α-converting enzyme catalytic domain (TCD) molecules.

55. (Amended) The method according to claim **[40]** **63**, wherein **the crystal of** said TNF-α-converting enzyme polypeptide **[crystal]** is of monoclinic space group $P2_1$ and the cell has the constants a=61.38 Å, b=126.27 Å, c=81.27 Å, and β=107.41°.

56. (Amended) The method according to claim **[40]** **63**, wherein the associating compound is designed to associate with the S1' region of TNF-α-converting enzyme.

57. (Amended) The method according to claim **[40]** **63**, wherein the associating compound is designed to associate with the S1'S3' pocket of TNF-α-converting enzyme.

58. (Amended) The method according to claim **[40]** **63**, wherein the associating compound is designed to incorporate a moiety that chelates zinc.

59. (Amended) The method according to claim **[40]** **63**, wherein the associating compound is designed to form a hydrogen bond with Leu348 or Gly349 of TNF-α-converting enzyme.